

Large Deviation Strategy for Inverse Problem

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Abstract

Taken traditionally as a no-go theorem against the theorization of inductive processes, Duhem-Quine thesis may interfere with the essence of statistical inference. This difficulty can be resolved by “Micro-Macro duality” [23, 24] which clarifies the importance of specifying the pertinent aspects and accuracy relevant to concrete contexts of scientific discussions and which ensures the matching between what to be described and what to describe in the form of the validity of duality relations. This consolidates the foundations of the inverse problem, induction method, and statistical inference crucial for the sound relations between theory and experiments. To achieve the purpose, we propose here Large Deviation Strategy (LDS for short) on the basis of Micro-Macro duality, quadrality scheme, and large deviation principle. According to the quadrality scheme emphasizing the basic roles played by the dynamics, algebra of observables together with its representations and universal notion of classifying space, LDS consists of four levels and we discuss its first and second levels in detail, aiming at establishing statistical inference concerning observables and states. By efficient use of the central measure, we will establish a quantum version of Sanov’s theorem, the Bayesian escort predictive state and the widely applicable information criteria for quantum states in LDS second level. Finally, these results are reexamined in the context of quantum estimation theory, and organized as quantum model selection, i.e., a quantum version of model selection.

1 Statistical Inference vs. Duhem-Quine Thesis

The main purpose of the present paper is to propose a general method for statistical inference which we call Large Deviation Strategy (LDS for short). To see the importance of this task, we first contrast it with the following famous dilemma of Duhem-Quine thesis. **Duhem-Quine thesis:** It is impossible to determine uniquely such a theory from phenomenological data as to reproduce the latter, because of unavoidable finiteness in number of measurable quantities and of their limited accuracy.

According to the standard interpretation of this thesis as a no-go theorem against the possibility of theorizing inductive processes, the communities of sciences (and philosophy of sciences) have long been dominated by such common and/or implicit consensus that the inductive aspects can be treated only in intuitive and heuristic manners without being incorporated into theories where only deductive arguments can be developed from some tentative and ad hoc starting postulates without satisfactory bases. In this situation,

we would totally lose any sound basis for the mutual connections between experimental and theoretical sides, by which any attempts for statistical estimates and inference would become meaningless. While this issue is seldom taken serious by working scientists such as physicists, the reason still remains to be explained why experimental sciences can work in spite of this no-go theorem; this question cannot be answered by the present-day forms of sciences (nor by philosophy of sciences) in the standard formulation, for lack of the theoretical elements of induction. Since “Macro” from the standard viewpoint of microscopic physics is nothing more than rough approximations of “Micro” levels, such important theoretical roles played by it as universal reference systems or its origin are hardly examined, and hence, no justification can be given of the status of “Macro”. In the light of the above Duhem-Quine thesis, therefore, it becomes evident not only that the sacred “Micro” theory itself in the usual approaches is just something postulated in an *ad hoc* way without any inevitable basis, for lack of the unique choices of theoretical starting points on the “Micro” side in relation to the “Macro” data, but also that the latter side is floating in the air without firm bases.

In sharp contrast, the formulation based on “Micro-Macro duality” [24] proposed by one of the authors (I.O.) resolves the above conflict in a natural way, on the basis of the duality between the “Micro” side to be described and the “Macro” side to describe. Therefore, it is necessary for the essence of “Micro-Macro duality” to be discussed .

1.1 Micro-Macro duality solving Duhem-Quine thesis and quadrality scheme

The notion of dualities can be formulated mathematically in its general form as categorical adjunctions [18] materializing the important aspects of mathematical universalities. In this context, “Micro” and “Macro” are interrelated with each other by “Micro-Macro duality” in bi-directional ways: “Macro” playing the roles of a standard reference frame is generated as a stabilized domain through the processes of emergence [26] from the dynamical motions in “Micro”. In the opposite direction, “Macro” \implies “Micro”, the extended machinery based on the so-called “dilation” method allows us to recover the original microscopic system, “Micro”, from phenomenological and/or experimental data in “Macro”, by means of such generalizations of the inverse Fourier transform as Tannaka-Krein-Tatsuuma duality [10, 17, 30, 31] and as Galois extensions materialized by crossed product formation [28]. In this way, the essence of the Micro-Macro duality can be understood as the adaptations to natural sciences of the mathematical notion of duality (or adjunction) appearing ubiquitously in mathematics.

What is most important here is the validity of mathematical universalities, which resolves the difficulties caused by the no-go theorem of Duhem-Quine thesis in the following way. According to the thesis, we cannot avoid any kind of indeterminacy on the phenomenological “Macro” side based on the statistical inference, because of the inevitable finiteness in number of measurable quantities and of their limited accuracy, which will lead to possible non-uniqueness of the results of inductions in the form of a theoretical starting point of “Micro” extracted from the phenomenological “Macro”. Because of the *universality* associated to “Micro-Macro duality”, the duality between “Micro” and “Macro”, the uniqueness of “Micro” is guaranteed *within the context* specified by the “Macro” in such forms as the relevant aspects and accuracies compatible with the phenomenological data.

In the standard approach in physics concentrating on the unilateral efforts to derive experimental predictions from theoretical hypotheses on the purely “Micro” side, this

kind of approach might be unfamiliar. So, we try to explain briefly the essence of some key notions relevant to duality. First, the notion of duality is widely applied in many mathematical contexts in such a form as the duality between an abstract group and (the totality of) its representations. One can also find duality in physics in such a form as position x and momentum p as it is essential for the basis of many concepts. The most typical example in the present context is the duality between observables and states. In the algebraic formulation of quantum theory, observables are defined as (self-adjoint) elements of a C^* -algebra, and states (or, called also expectation values) as normalized positive linear functionals on the algebra of observables. A simple example of this sort is given by the well-known Gel'fand isomorphism between a commutative C^* -algebra and a Hausdorff space as its spectrum. In more detail, denoting the categories of commutative C^* -algebras and of Hausdorff spaces, respectively, by $CommC^*Alg$ and $HausSp$, we have the following isomorphic relations between the relevant morphisms in the two categories for $\mathfrak{A} \in CommC^*Alg$, $M \in HausSp$,

$$CommC^*Alg(\mathfrak{A}, C_0(M)) \simeq HausSp(M, Spec(\mathfrak{A})), \quad (1)$$

where $C_0(M)$ is the commutative C^* -algebra consisting of functions on M vanishing at infinity, and $Spec(\mathfrak{A}) := \{\chi : \mathfrak{A} \rightarrow \mathbb{C} \mid \chi: \text{character satisfying } \chi(AB) = \chi(A)\chi(B) \text{ for } A, B \in \mathfrak{A}\}$. The isomorphism \simeq is determined by the equality $[\varphi^*(x)](A) = [\varphi(A)](x)$ for a $*$ -homomorphism $\varphi : \mathfrak{A} \rightarrow C_0(M)$ and its dual map $\varphi^* : M \rightarrow Spec(\mathfrak{A})$. When $M = Spec(\mathfrak{A})$, this reduces to the identification, $\mathfrak{A} \simeq C_0(Spec(\mathfrak{A}))$, between an abstract commutative C^* -algebra \mathfrak{A} and a concrete commutative C^* -algebra $C_0(Spec(\mathfrak{A}))$ of continuous functions on $Spec(\mathfrak{A})$ through the relation $\mathfrak{A} \ni A \longleftrightarrow \hat{A} \in C_0(Spec(\mathfrak{A}))$ defined by $\chi(A) = \hat{A}(\chi)$, $\chi \in Spec(\mathfrak{A})$. In this connection, a state as an expectation value can be shown just to correspond to a probability measure according to Markov-Kakutani theorem [5], which involves already such a statistical aspect as i.i.d. property as will be shown later. Other examples are given as follows:

Example 1.1. *A finite-dimensional vector space V is isomorphic with its second dual V^{**} :*

$$V \cong V^{**}. \quad (2)$$

Example 1.2. *Let G be a locally compact abelian group. Its dual group \hat{G} defined by the set of unitary characters on G is also a locally compact abelian group w.r.t. the pointwise product. Furthermore, $\widehat{(\hat{G})} =: \hat{\hat{G}}$, called the second dual group, can be defined and the following relation, called Pontryagin duality, holds:*

$$\hat{\hat{G}} \cong G, \quad (3)$$

as topological groups.

In statistics also, duality is known to play essential roles: the Riemannian geometric formulation of statistics is called information geometry [4] and based on a duality structure. For any $\alpha \in \mathbb{R}$, the α -connection is defined on the Riemannian manifold consisting of a family of probability distributions and has the dual connection corresponding to the $(-\alpha)$ -connection. The α -connection determines the unique quasi-distance of probability distributions, called an α -divergence, which generalizes the Kullback-Leibler divergence. Thus the duality is seen to play essential roles in various contexts.

To consolidate the natural inter-relations between experiments and theories, and between “Macro” and “Micro”, we proceed further to a theoretical framework based on

the Micro-Macro duality. In terms of the four basic ingredients closely related to the representation-theoretical context of dynamical systems, a coherent scheme for theoretical description of a target system of our recognition can be formulated as a pair of duality pairs, which we call a quadrality scheme [25]:

$$\begin{array}{ccc}
 \text{Macro} & & 3. \text{ Spectrum } (Spec) \\
 2. \text{ States } (State) \text{ and} & \Leftrightarrow & 1. \text{ Algebra } (Alg) . \\
 \text{Representations } (Rep) & & \\
 & 4. \text{ Dynamics } (Dyn) & \text{Micro}
 \end{array}$$

Here, the dynamics (Dyn) at the bottom creates an algebra (Alg) of observables to characterize an object system, and the configurations or structures of the objects in (Alg) are described mathematically in terms the notion of states (as interfaces between Micro and Macro) and the associated (GNS-)representations of (Alg) which we denote by (Rep). Roughly speaking, “Micro” corresponds to a dynamical system consisting of (Dyn) and (Alg), and “Macro” to a (co)dynamical one of (Rep) and (Spec). In the direction from “Macro” to “Micro”, we find two arrows, one from the experimental side to the theoretical one in the form of induction processes, and another in the operational contexts of controls over the system under consideration, which should include the aspect of the state preparation indispensable in conducting experiments. The former one, induction, is materialized usually on the basis of statistical inference, in combination with suitable choices of classification schemes. The aspects of control theory and state preparation are strongly interrelated.

To materialize an induction scheme, we should combine the large deviation principle (LDP for short) as the mathematical core of statistical inference with the above quadrality scheme in view of its essential roles in implementing “Micro-Macro duality” indispensable for overcoming the Duhem-Quine no-go theorem. From this viewpoint, we propose in Section 2 Large Deviation Strategy as a systematic method of induction, where the importance of statistical inference is emphasized. Here statistical estimation is no more than the method to analyze several ingredients such as means, probability distributions and coefficients of stochastic differential equations, and is fundamentally based on LDP extended by the quadrality scheme. Stein’s lemma and Chernoff bounds in hypothesis testing are the typical examples in this context. All these discussions explain the reason why we adopt such naming as Large Deviation Strategy. After briefly mentioning in Section 3 two example cases of the application of LDS, we clarify in Section 4 the meaningful and precise relations between quantum and classical levels in the context of estimation theory, especially concerning the problem of model selection. In Appendix, the operational meaning of Tomita’s theorem of barycentric decomposition crucial for the second level of LDS is explained from the viewpoint of a measurement process. In this way, the theoretical bases of LDS can be found in Micro-Macro duality [24], quadrality scheme and LDP extended by the quadrality scheme. Before going into LDS, it will be instructive to explain the mutual relations among the relevant tools:

1.2 Interdependence among statistical inference, Micro-Macro duality, quadrality scheme and LDS

The logical relations among the three items including LDS itself is actually a kind of mutual interdependence in the following sense:

- i) statistical inference \implies Micro-Macro duality: as Micro-Macro duality is based on

the duality between the inductive and deductive arguments, it is not possible without the reliable methods and schemes for statistical inference.

ii) Micro-Macro duality \implies quadrality scheme: The duality between (Alg) and (Rep) guarantees the matching between what is to be described in (Alg) and what to describe by (Rep), which is just the most important step to resolve the difficulties caused by the no-go theorem of Duhem-Quine thesis mentioned at the beginning. To attain a meaningful *interpretation* from the items obtained above, we need to apply some *classification* to the states and representations in (Rep) according to some relevant viewpoints, as a result of which we can attain the level of (Spec) containing all the *classifying parameters* to specify each configuration realized in (Rep). Then the validity of duality between (Spec) and (Dyn) allows a universal parametrization of the dynamics, (Dyn), of the object system in terms of the parameters belonging to (Spec), whose special case can be found in the familiar parametrization of dynamical map $t \mapsto \alpha_t$ in terms of a time parameter $t \in \mathbb{R}$.

iii) quadrality scheme \implies (an extended form of) LDP: the standard application of LDP starts from the calculation of a rate function to measure deviations of empirical data of an observable from its “true” value (of its average), which is sometimes called the LDP at the first level [9]. In view of ii) above, this corresponds to discussing (Alg) (or, more precisely, a subalgebra of (Alg) generated by the specific observable under consideration). For the purpose of statistical inference, however, what is most relevant is that of such a state as generating a certain definite pattern of empirical data, like the case of a quantum state yielding a statistical ensemble allowing the Born formula. This requires us to proceed from (Alg) to (Rep) in the quadrality scheme in ii) in the context of LDP, which constitutes the main contents of Sec. 2.3. We try further to extend the scheme to incorporate the level of (Spec) which enables us to deform and adjust the choice of model spaces in an optimal way and which we call the LDP third level. Once this is achieved, we can further proceed to the inference of the dynamical law (Dyn) of the system under consideration, taking advantage of the duality between (Spec) and (Dyn), which can be called the LDP fourth level.

iv) extended LDP \implies LDS: LDS can be obtained by applying the above extended scheme of LDP to the context of statistical inference, by means of which we can attain a full-fledged form of the latter, and hence, we can re-start i). This loop structure can be easily organized into a helical or spiral form to deepen the levels of our theoretical descriptions.

2 Large Deviation Strategy

2.1 What is Large Deviation Strategy?

Now, our Large Deviation Strategy (LDS) is a method of statistical inference by step-by-step inductions according to the basic idea constituting the large deviation principle (LDP). We suppose that LDS consists of the following four levels just in parallel with LDP in its extended form:

1st level : Abelian von Neumann algebras

Gel’fand representation, Strong law of large numbers(SLLN)
and statistical inference on abelian von Neumann algebras

2nd level : *States* and *Reps*

3rd level : *Spec* and *Alg*

Emergence of space-time from composite systems
of internal and external degrees of freedom

4th level : *Dyn* From emergence to space-time patterns and time-series analysis

The aim of the first level is to estimate the spectra of observables and their probability distributions. If we restrict our attention to mutually consistent observables, this is equivalent to considering the problem to estimate a spectrum of *abelian von Neumann subalgebra* generated by the mutually commuting observables. The obtained information at this stage should help us to restrict the class of states and representations relevant to the second level, the latter of which aims at the estimate of states and the associated representations defined on the algebra of all observables. To proceed to the third level, we consider a composite system consisting of the object system to be described and of the macroscopic degrees of freedom arising from the processes of emergence from the microscopic ones. At the fourth level, we consider the estimate of the dynamics of the system which will allow us to proceed to the stage of controlling the object system. The following methods will play central roles in LDS:

I. Large deviation principle [7, 9]:

From probabilistic fluctuations to statistical inference

II. Tomita decomposition theorem and central decomposition:

To formulate and use state-valued random variables

III. The dual \widehat{G} of a group G and its crossed products:

To reconstruct Micro from the data of Macro

IV. Emergence: Condensation associated with spontaneous symmetry

breaking (SSB) and phase separation in the direction from Micro to Macro

LDP works effectively at each level of our strategy and provides us with the information of rate functions in such forms as free energy and relative entropy, for instance. This information clarifies to which extent a given quantity in question can deviate from its fiducial point which is called the “true” value. In this way, LDP is seen to be essential for statistical inference. As discussed in Sec.2.3, the notion of state-valued random variables can successfully be formulated in the use of Tomita decomposition theorem and central decompositions. In the second level where states and representations are estimated, this formulation enables us to analyze them in terms of “numerical” data. We can also see the necessity of the items in the above III and the processes of emergence in the third level (in reference to [26] and to the discussion in the previous section).

2.2 1st Level: Observables and Abelian Subalgebra

As stated in the previous subsection, we discuss here the mean and the probability distribution of an observable. Let \mathfrak{A} be a C^* -algebra, ψ be a state (defined as a normalized positive linear functional) on \mathfrak{A} and A be an observable to be measured which is identified by an element of \mathfrak{A} . \mathcal{A} denotes the abelian subalgebra of \mathfrak{A} generated by A , and states on \mathfrak{A} is naturally restricted to \mathcal{A} . Therefore, we try to estimate the appropriate pair $(A, \psi|_{\mathcal{A}})$. The candidate of A comes from the following theorem.

Theorem 2.1. *An abelian von Neumann algebra \mathfrak{M} on a separable Hilbert space \mathfrak{H} is generated by one element X (belonging to \mathfrak{M}).*

If X is selfadjoint, then we put $A = X$.

For an abelian von Neumann algebra \mathcal{A} and ψ a normal state on \mathcal{A} , the following relations hold:

$$\begin{aligned}\langle \Omega_\psi, \pi_\psi(A) \Omega_\psi \rangle &= \psi(A) = \int \hat{A}(k) d\nu_\psi(k), \\ \pi_\psi(\mathcal{A}) \ni \pi_\psi(A) &\longleftrightarrow \hat{A} \in L^\infty(K, \nu_\psi), \\ \mathfrak{H}_\psi &\cong L^2(K, \nu_\psi) \\ (\mathfrak{H}_\psi \ni \Omega_\psi &\longleftrightarrow 1 \in L^2(K, \nu_\psi)), \\ \mathcal{A}_* &\cong L^1(K, \nu_\psi),\end{aligned}$$

where K is a compact Hausdorff space and ν_ψ is a Borel measure on K . Every self-adjoint element $\pi_\psi(A)$ of $\pi_\psi(\mathcal{A})$ is treated as measure-theoretical \mathbb{R} -valued random variable \hat{A} . Thus, we can discuss spectra of observables in the commutative case.

For any $\bar{k} = (k_1, k_2, \dots) \in K^\mathbb{N}$ and $A = A^* \in \mathcal{A}$, we define $X_j(\bar{k}) = k_j$ and $\hat{A}_j(\bar{k}) := \hat{A}(X_j(\bar{k}))$, we see the validity of

Matching Condition 1. *$\{\hat{A}_j\}$ are independent identically distributed (“i.i.d.”) random variables.*

For any measure m , let $P_m := m^\mathbb{N}$ denote the product measure of m defined by a countably many tensor power. The following theorem is known to hold:

Theorem 2.2 (Cramér’s theorem [7]). *Let $M_n(\bar{k}) := \frac{1}{n}(\hat{A}_1(\bar{k}) + \dots + \hat{A}_n(\bar{k}))$ and $Q_n^{(1)}(\Gamma) := P_{\nu_\psi}(M_n \in \Gamma)$. Then, $Q_n^{(1)}$ satisfies LDP with the rate function $I_\psi(a) = \sup_{t \in \mathbb{R}} \{at - c_\psi(t)\}$ ($c_\psi(t) = \log \int_{\mathbb{R}} e^{tx} \nu_\psi(\hat{A} \in dx)$):*

$$\begin{aligned}- \inf_{a \in \Gamma^o} I_\psi(a) &\leq \liminf_{n \rightarrow \infty} \frac{1}{n} \log Q_n^{(1)}(\Gamma) \\ &\leq \limsup_{n \rightarrow \infty} \frac{1}{n} \log Q_n^{(1)}(\Gamma) \leq - \inf_{a \in \overline{\Gamma}} I_\psi(a)\end{aligned}\tag{4}$$

By this theorem, we can discuss the convergence rate of the arithmetic means of observables and estimate “true” means.

As the next step, we give a satisfactory formulation for estimating probability distributions.

Definition 2.1. A family of probability distributions $\{p(x|w)|w \in W\}$ (with a compact set $W \subset \mathbb{R}^l$) is called a (statistical) model if it satisfies the condition that the set $\{x \in \mathbb{R}^d | p(x|w) > 0\}$ is independent of $w \in W$.

Definition 2.2. The probability distribution $p_{\pi,\beta}(x|x^n)$ defined below is called a Bayesian escort predictive distribution:

$$p_{\pi,\beta}(x|x^n) = \langle p(x|w) \rangle_{\pi,\beta}^{x^n} = \frac{\int p(x|w) \prod_{j=1}^n p(x_j|w)^\beta \pi(w) dw}{\int \prod_{j=1}^n p(x_j|w)^\beta \pi(w) dw}, \quad (5)$$

where $\pi(w)$ is a probability distribution (p.d., for short) on W and $\beta > 0$.

We denote by $M_1(\Sigma)$ the space of Borel probability measures on a Polish space Σ . We define the relative entropy of the probability measure $\nu \in M_1(\Sigma)$ with respect to $\mu \in M_1(\Sigma)$ as

$$D(\nu||\mu) = \begin{cases} \int d\nu(\rho) \log \frac{d\nu}{d\mu}(\rho) & (\nu \ll \mu) \\ +\infty & (\text{otherwise}). \end{cases} \quad (6)$$

If there exists a probability measure $\sigma \in M_1(\Sigma)$ such that $\nu, \mu \ll \sigma$, $D(\nu||\mu)$ is also denoted by $D(q||p)$ where $q := \frac{d\nu}{d\sigma}$ and $p := \frac{d\mu}{d\sigma}$.

Theorem 2.3. For $r(\cdot|x^n)$ as a p.d.-valued function $x^n = \{x_1, \dots, x_n\} \mapsto r(\cdot|x^n)$, its risk function $\mathcal{R}^n(p||r)$ defined by

$$\mathcal{R}^n(p||r) = \iint D(p(\cdot|w)||r(\cdot|x^n)) \prod_{j=1}^n p(x_j|w)^\beta dx_j \pi(w) dw \quad (7)$$

is minimized by the Bayesian escort predictive distribution $p_{\pi,\beta}(x|x^n)$.

Proof. See [1, 33]. □

While there are some more items to be treated in statistical inference, those appearing in the next subsection are essentially all what we need in the second level.

2.3 2nd Level: States and Representations

In order to proceed to the second level where states of the algebra of observables are the target to be evaluated, we need to prepare certain advanced operator-algebraic setting which is provided by Tomita's theorem of integral decomposition of states. For the purpose, we first review the notion of sectors. For a C*-algebra \mathfrak{A} let $E_{\mathfrak{A}}$ be the set of its states defined by normalized positive linear functionals on \mathfrak{A} . A state $\omega \in E_{\mathfrak{A}}$ is called a factor state if the von Neumann algebra $\pi_{\omega}(\mathfrak{A})''$ corresponding to the GNS representation $\{\mathfrak{H}_{\omega}, \pi_{\omega}\}$ is a factor with a trivial center: $\mathfrak{Z}_{\omega}(\mathfrak{A}) := \pi_{\omega}(\mathfrak{A})'' \cap \pi_{\omega}(\mathfrak{A})' = \mathbb{C}1_{\mathfrak{H}_{\omega}}$. We denote by $F_{\mathfrak{A}}$ the set of all factor states of \mathfrak{A} . If π is a representation of \mathfrak{A} , then a state ω of \mathfrak{A} is said to be π -normal if there exists a normal state ρ of $\pi(\mathfrak{A})''$ such that

$$\omega(A) = \rho(\pi(A)) \quad (8)$$

for all $A \in \mathfrak{A}$. Two representations π_1 and π_2 of a C*-algebra \mathfrak{A} are said to be quasi-equivalent and written as $\pi_1 \approx \pi_2$, if each π_1 -normal state is π_2 -normal and vice versa.

Definition 2.3 ([23]). A sector of C^* -algebra \mathfrak{A} is defined by a quasi-equivalence class of factor states of \mathfrak{A} .

If $\{\pi, \mathfrak{H}\}$ is a representation of a C^* -algebra \mathfrak{A} , and n is a cardinal, let $n\pi$ denote the representation of \mathfrak{A} on $\mathfrak{H}^{\oplus n} = \bigoplus_{k=1}^n \mathfrak{H}$ defined by

$$n\pi(A) \left(\bigoplus_{k=1}^n \xi_k \right) = \bigoplus_{k=1}^n (\pi(A)\xi_k). \quad (9)$$

By the following standard theorem in the representation theory of operator algebras, quasi-equivalence between two representations π_1 and π_2 can be seen as the isomorphism between the corresponding von Neumann algebras, $\pi_1(\mathfrak{A})''$ and $\pi_2(\mathfrak{A})''$, or as the unitary equivalence of π_1 and π_2 up to multiplicity:

Theorem 2.4 (see [5]). Let \mathfrak{A} be a C^* -algebra and let $\{\pi_1, \mathfrak{H}_1\}$ and $\{\pi_2, \mathfrak{H}_2\}$ be nondegenerate representations of \mathfrak{A} . The following are equivalent:

- (1) $\pi_1 \approx \pi_2$;
- (2) there exists an isomorphism $\tau : \pi_1(\mathfrak{A})'' \mapsto \pi_2(\mathfrak{A})''$ such that $\tau(\pi_1(A)) = \pi_2(A)$ for all $A \in \mathfrak{A}$;
- (3) there exist cardinals n, m , projections $E \in n\pi_1(\mathfrak{A})'$, $F \in n\pi_2(\mathfrak{A})'$ and unitary elements $U : \mathfrak{H}_1 \mapsto F(\mathfrak{H}_2^{\oplus m})$, $V : \mathfrak{H}_2 \mapsto E(\mathfrak{H}_1^{\oplus n})$ such that

$$\begin{aligned} U\pi_1(A)U^* &= m\pi_2(A)F, \\ V\pi_2(A)V^* &= n\pi_1(A)E \end{aligned}$$

for all $A \in \mathfrak{A}$;

- (4) There exists a cardinal n such that $n\pi_1 \cong n\pi_2$, i.e., π_1 and π_2 are unitary equivalent up to multiplicity.

The Gel'fand spectrum $\text{Spec}(\mathfrak{Z}_\omega(\mathfrak{A}))$ of the center $\mathfrak{Z}_\omega(\mathfrak{A})$ is then identified with a factor spectrum $\widehat{\mathfrak{A}}$ of \mathfrak{A} :

$$\text{Spec}(\mathfrak{Z}_\omega(\mathfrak{A})) \cong \widehat{\mathfrak{A}} := F_{\mathfrak{A}}/\approx : \text{factor spectrum}.$$

The center $\mathfrak{Z}_\omega(\mathfrak{A})$ and the factor spectrum $\widehat{\mathfrak{A}}$ play the role of the abelian algebra of macroscopic order parameters to specify sectors and the classifying space of sectors to distinguish among different sectors, respectively [23].

As already mentioned, we need to treat states as objects to be estimated in the second level of LDP, which means the necessity for “states to be treated as observables”. The notion of state-valued random variables required for this purpose can successfully be formulated in the use of Tomita’s theorem for orthogonal decompositions of states by barycentric orthogonal measures whose special case of central decompositions [22, 23] is seen to be particularly useful for our purposes of statistical inference of state estimate. Now the orthogonality $\omega_1 \perp \omega_2$ of positive linear functionals $\omega_i \in \mathfrak{A}_+^*$ and the orthogonal measures μ on the state space $E_{\mathfrak{A}}$ of a C^* -algebra \mathfrak{A} are defined, respectively, as follows (see [5]):

Definition 2.4. If $\omega_1, \omega_2 \in \mathfrak{A}_+^*$ satisfy any of the following three equivalent conditions, they are said to be orthogonal and we write $\omega_1 \perp \omega_2$:

1. if $\omega' \leq \omega_1$ and $\omega' \leq \omega_2$ for $\omega' \in \mathfrak{A}_+^*$ then $\omega' = 0$;
2. there is a projection $P \in \pi_\omega(\mathfrak{A})'$ s.t. $\omega_1(A) = \langle P\Omega_\omega, \pi_\omega(A)\Omega_\omega \rangle$ and $\omega_2(A) = \langle (1 - P)\Omega_\omega, \pi_\omega(A)\Omega_\omega \rangle$;
3. the representation associated to $\omega = \omega_1 + \omega_2$ is a direct sum of the representations associated with ω_1 and ω_2 ,

$$\mathfrak{H}_\omega = \mathfrak{H}_{\omega_1} \oplus \mathfrak{H}_{\omega_2}, \quad \pi_\omega = \pi_{\omega_1} \oplus \pi_{\omega_2}, \quad \Omega_\omega = \Omega_{\omega_1} \oplus \Omega_{\omega_2}.$$

Definition 2.5. A positive regular Borel measure μ on $E_{\mathfrak{A}}$ is defined to be an orthogonal measure on $E_{\mathfrak{A}}$ if it satisfies for any Borel set $S \subset E_{\mathfrak{A}}$ the condition

$$\left(\int_S \rho \, d\mu(\rho) \right) \perp \left(\int_{E_{\mathfrak{A}} \setminus S} \rho \, d\mu(\rho) \right). \quad (10)$$

The important properties characteristic to these notions can be found in the following theorem due to Tomita:

Theorem 2.5 (Tomita's theorem, see [5]). *Let \mathfrak{A} be a C^* -algebra and ω be a state on \mathfrak{A} . There exists one-to-one correspondence between the following three sets:*

- (1) the orthogonal measures μ with barycenter $\omega = \int_{E_{\mathfrak{A}}} \rho d\mu(\rho)$;
- (2) the abelian von Neumann subalgebras $\mathfrak{B} \subseteq \pi_\omega(\mathfrak{A})'$;
- (3) the orthogonal projections P on \mathfrak{H}_ω such that

$$P\Omega_\omega = \Omega_\omega, \quad P\pi_\omega(\mathfrak{A})P \subseteq \{P\pi_\omega(\mathfrak{A})P\}'$$

If μ, \mathfrak{B}, P are in correspondence one has the following relations:

- (1) $\mathfrak{B} = \{\pi_\omega(\mathfrak{A}) \cup P\}'$; (2) $P = [\mathfrak{B}\Omega_\omega]$;
- (3) $\mu(\hat{A}_1 \hat{A}_2 \cdots \hat{A}_n) = \langle \Omega_\omega, \pi_\omega(A_1)P\pi_\omega(A_2)P \cdots P\pi_\omega(A_n)\Omega_\omega \rangle$;
- (4) \mathfrak{B} is $*$ -isomorphic to the range of the map $L^\infty(\mu) := L^\infty(E_{\mathfrak{A}}, \mu) \ni f \mapsto \kappa_\mu(f) \in \pi_\omega(\mathfrak{A})'$ defined by

$$\langle \Omega_\omega, \kappa_\mu(f)\pi_\omega(A)\Omega_\omega \rangle = \int_{E_{\mathfrak{A}}} f(\rho) \hat{A}(\rho) d\mu(\rho) \quad (11)$$

and for $A, B \in \mathfrak{A}$

$$\kappa_\mu(\hat{A})\pi_\omega(B)\Omega_\omega = \pi_\omega(B)P\pi_\omega(A)\Omega_\omega, \quad (12)$$

where the map $\mathfrak{A} \ni A \mapsto \hat{A} \in L^\infty(\mu)$ is defined by $\hat{A} := (E_{\mathfrak{A}} \ni \rho \mapsto \rho(A))$.

The above measure μ is called a barycentric measure of the state ω , which is, in turn, called the barycenter $\omega = b(\mu) := \int_{E_{\mathfrak{A}}} \rho \, d\mu(\rho)$ of μ . The set of orthogonal probability measures μ on $E_{\mathfrak{A}}$ with barycentre ω is denoted by $\mathcal{O}_\omega(E_{\mathfrak{A}})$. In reference to the abelian von Neumann algebra \mathfrak{B} , we also denote the measure μ by $\mu_{\mathfrak{B}}$. We add here the following observation to extend the essential contents of the Gel'fand isomorphism for commutative C^* -algebras to the non-commutative situation: the image $\hat{\mathfrak{A}} := \{\hat{A} | A \in \mathfrak{A}\}$ of the map $\mathfrak{A} \ni A \mapsto \hat{A} \in L^\infty(\mu)$ is contained in the universal enveloping von Neumann algebra \mathfrak{A}^{**} of \mathfrak{A} and constitutes a C^* -algebra of measure-theoretical random variables equipped with a linear structure $(\alpha\hat{A} + \beta\hat{B})(\rho) := (\alpha\hat{A} + \beta\hat{B})(\rho)$ ($\alpha, \beta \in \mathbb{C}$), a non-commutative convolution product defined by $(\hat{A} * \hat{B})(\rho) := \widehat{AB}(\rho)$, and the norm $\|\cdot\|$ given by

$$\|\hat{A}\| = \sup_{\substack{\rho \in E_{\mathfrak{A}}, \\ \|\rho\|=1}} |\hat{A}(\rho)|. \quad (13)$$

Definition 2.6. If the algebra \mathfrak{B} corresponding to μ is a subalgebra of the center $\mathfrak{Z}_\omega(\mathfrak{A})$ of the GNS representation π_ω of ω , the orthogonal measure $\mu = \mu_{\mathfrak{B}} \in \mathcal{O}_\omega(E_{\mathfrak{A}})$ is called a subcentral measure of ω satisfying the condition that, for any Borel set $\Delta \subset E_{\mathfrak{A}}$, the pair of subrepresentations, $\int_{\Delta}^{\oplus} \pi_\rho d\mu(\rho)$ and $\int_{E_{\mathfrak{A}} \setminus \Delta}^{\oplus} \pi_\rho d\mu(\rho)$, of π_ω are disjoint in the sense of the absence of non-zero intertwiners. In the case of $\mathfrak{B} = \mathfrak{Z}_\omega(\mathfrak{A})$, the corresponding subcentral measure is called the central measure of ω and denoted by $\mu_\omega := \mu_{\mathfrak{Z}_\omega(\mathfrak{A})} \in \mathcal{O}_\omega(E_{\mathfrak{A}})$.

Since κ_{μ_ω} is a $*$ -algebraic embedding of $L^\infty(\mu)$, we can define a projection-valued measure (PVM) $E_\omega : (\mathfrak{B}(\text{supp } \mu_\omega) \ni \Delta \mapsto E_\omega(\Delta) \in \text{Proj}(\mathfrak{Z}_\omega(\mathfrak{A})))$ on Borel subsets $\Delta \in \mathfrak{B}(\text{supp } \mu_\omega)$ of the state space $E_{\mathfrak{A}}$ by $E_\omega(\Delta) := \kappa_{\mu_\omega}(\chi_\Delta) \in \text{Proj}(\mathfrak{Z}_\omega(\mathfrak{A}))$, which satisfies

$$\langle \Omega_\omega, E_\omega(\Delta) \Omega_\omega \rangle = \mu_\omega(\Delta). \quad (14)$$

Here the indicator function χ_Δ for a subset Δ of $E_{\mathfrak{A}}$ is defined as usual:

$$\chi_\Delta(\rho) = \begin{cases} 1 & (\rho \in \Delta), \\ 0 & (\rho \notin \Delta). \end{cases}$$

In this way, states ρ on $\text{supp}(\mu_\omega)$ constitute a random variable on the central spectrum, and each element $\kappa_{\mu_\omega}(f) \in \kappa_{\mu_\omega}(L^\infty(\mu_\omega)) = \mathfrak{B} = \mathfrak{Z}_\omega(\mathfrak{A})$ can be expressed as

$$\kappa_{\mu_\omega}(f) = \int f(\rho) dE_\omega(\rho). \quad (15)$$

Therefore, the center $\mathfrak{Z}_\omega(\mathfrak{A})$ of \mathfrak{A} can be seen as an algebra consisting of non-linear functions of states.

When the methods discussed in this section are applied to practical situations, it will be safe and also sufficient for us to restrict ourselves to such cases that the support of the barycentric measure μ_ω is a compact subset B in the factor spectrum $F_{\mathfrak{A}}$ of \mathfrak{A} :

$$\omega = \int \rho d\mu_\omega(\rho) = \int_B \rho_\xi d\tilde{\mu}(\xi) \quad (16)$$

where $\{\rho_\xi | \xi \in \Xi : \text{an order parameter}\} \subset F_{\mathfrak{A}}$. Here the factor spectrum $F_{\mathfrak{A}}$ of \mathfrak{A} means the subset of the state space $E_{\mathfrak{A}}$ consisting of all the factor states φ whose GNS representations have trivial centers: $\mathfrak{Z}_\varphi(\mathfrak{A}) = \pi_\varphi(\mathfrak{A})'' \cap \pi_\varphi(\mathfrak{A})' = \mathbb{C}1_{\mathfrak{H}_\varphi}$.

2.3.1 Mathematical and statistical basis

Let \mathfrak{A} be a separable C^* -algebra and ψ be a state on \mathfrak{A} . Then $E_{\mathfrak{A}}$ is weak $*$ -compact and metrizable by the metric

$$d(\omega_1, \omega_2) = \sum_{j=1}^{\infty} \frac{1}{2^j} \frac{|\omega_1(A_j) - \omega_2(A_j)|}{\|A_j\|}, \quad (17)$$

where the set $\{A_j \in \mathfrak{A} | A_j \neq 0, j = 1, 2, \dots\}$ is a dense subset of $E_{\mathfrak{A}}$. Thus $\text{supp } \mu_\psi$ of the central measure μ_ψ of $\psi \in E_{\mathfrak{A}}$ is compact in the weak $*$ -topology and $(\text{supp } \mu_\psi)^\mathbb{N}$ is also compact by Tikhonov's theorem. For $\tilde{\rho} = (\rho_1, \rho_2, \dots) \in (\text{supp } \mu_\psi)^\mathbb{N}$, we define $Y_j(\tilde{\rho}) = \rho_j$. Each ρ_j is a factor state because μ_ψ is supported by the closed subset of $F_{\mathfrak{A}}$, the set of factor states. Then $\{Y_j\}_{j=1}^\infty$ is seen to be a set of $(\text{supp } \mu_\psi)$ -valued random variables satisfying the following condition:

Matching Condition 2. $\{Y_j\}$ are independent identically distributed (“i.i.d.”) random variables.

We denote by $M_1(\Sigma)$ the space of Borel probability measures on a Polish space Σ , and by $B(\Sigma)$ the vector space of all bounded Borel measurable functions on Σ , respectively. For $\phi \in B(\Sigma)$, let $\tau_\phi : M_1(\Sigma) \rightarrow \mathbb{R}$ be defined by $\tau_\phi(\nu) = \langle \phi, \nu \rangle = \int_\Sigma \phi d\nu$. We denote by $\mathcal{B}_{cy}(M_1(\Sigma))$ the σ -field of cylinder sets on $M_1(\Sigma)$, i.e., the smallest σ -field that makes all $\{\tau_\phi\}$ measurable (see [7]).

For any $\tilde{\rho} \in (\text{supp } \mu_\psi)^\mathbb{N}$, $A \in \mathcal{B}(\text{supp } \mu_\psi)$ and $\Gamma \in \mathcal{B}_{cy}(M_1(E_\mathfrak{A}))$, we define the empirical measures

$$L_n(\tilde{\rho}, A) = \frac{1}{n} \sum_{j=1}^n \delta_{Y_j(\tilde{\rho})}(A), \quad (18)$$

and

$$Q_n^{(2)}(\Gamma) = P_{\mu_\psi}(L_n \in \Gamma). \quad (19)$$

The next theorem [14] is the key to proving LDP:

Theorem 2.6 (HOT83). *Let μ, ν be regular Borel probability measures on $E_\mathfrak{A}$ with barycenters $\omega, \psi \in E_\mathfrak{A}$. If there is a subcentral measure m on $E_\mathfrak{A}$ such that $\mu, \nu \ll m$, then $S(\psi||\omega) = D(\nu||\mu)$.*

This theorem enables us to evaluate the quantum relative entropy $S(\psi||\omega)$ as the measure-theoretical relative entropy $D(\nu||\mu)$.

Theorem 2.7. *Let \mathfrak{A} be a separable C^* -algebra and ψ be a state on \mathfrak{A} . Then $Q_n^{(2)}$ satisfies LDP with the rate function $S(b(\cdot)||\psi)$:*

$$-\inf_{\nu \in \Gamma^o, \nu \ll \mu_\psi} S(b(\nu)||\psi) \leq \liminf_{n \rightarrow \infty} \frac{1}{n} \log Q_n^{(2)}(\Gamma) \leq \limsup_{n \rightarrow \infty} \frac{1}{n} \log Q_n^{(2)}(\Gamma) \leq -\inf_{\nu \in \bar{\Gamma}, \nu \ll \mu_\psi} S(b(\nu)||\psi) \quad (20)$$

for any $\Gamma \in \mathcal{B}_{cy}(M_1(E_\mathfrak{A}))$. In the case that, for $\Gamma \in \mathcal{B}_{cy}(M_1(E_\mathfrak{A}))$, $\{\nu \in \Gamma^o | \nu \ll \mu_\psi\}$ and $\{\nu \in \bar{\Gamma} | \nu \ll \mu_\psi\}$ are empty, $\inf_{\nu \in \Gamma^o, \nu \ll \mu_\psi} S(b(\nu)||\psi)$ and $\inf_{\nu \in \bar{\Gamma}, \nu \ll \mu_\psi} S(b(\nu)||\psi)$ are defined as infinity, respectively.

Proof. $(E_\mathfrak{A}, d)$ with the metric d defined by (17) is a compact metric space, so is a Polish one. Therefore, we can apply Sanov’s theorem [7] for $Q_n^{(2)}(\Gamma)$ to prove this theorem by using Theorem 2.6 (HOT83). \square

In Appendix A a generalization of this theorem will be discussed, but we should first justify the use of generic barycentric measures in the context of statistical inference.

Definition 2.7. *A family of states $\{\omega_\theta | \theta \in \Theta\}$ parametrized by a compact set Θ in \mathbb{R}^d is called a (statistical) model if it satisfies the following three conditions:*

(i) *There is a subcentral measure m on $E_\mathfrak{A}$ such that $\mu_{\omega_\theta} \ll m$ for every $\theta \in \Theta$.*

(ii) *The set $\left\{ \rho \in E_\mathfrak{A} \middle| p_\theta := \frac{d\mu_{\omega_\theta}}{dm}(\rho) > 0 \right\}$ is independent of $\theta \in \Theta$.*

(iii) *ω_θ is Bochner integrable.*

Definition 2.8. For a given model $\{\omega_\theta\}_{\theta \in \Theta}$, a probability distributions $\pi(\theta)$ of θ , a state $\omega_{\pi, \beta}^n$ defined by

$$\omega_{\pi, \beta}^n := \frac{\int \omega_\theta \prod_{j=1}^n p_\theta(\rho_j)^\beta \pi(\theta) d\theta}{\int \prod_{j=1}^n p_\theta(\rho_j)^\beta \pi(\theta) d\theta} \quad (21)$$

is called a Bayesian escort predictive state, where $\rho^n := \{\rho_1, \dots, \rho_n\}$ and $\beta > 0$.

We obtain the following important theorem:

Theorem 2.8. For ϕ^{ρ^n} as a state-valued function $\rho^n = \{\rho_1, \dots, \rho_n\} \mapsto \phi^{\rho^n} \in E_{\mathfrak{A}}$, its risk function $T^n(\omega_\theta \| \phi^{\rho^n})$ defined by

$$T^n(\omega_\theta \| \phi^{\rho^n}) := \frac{1}{A} \iint S(\omega_\theta \| \psi^{\rho^n}) \prod_{j=1}^n p_\theta(\rho_j)^\beta dm(\rho_j) \pi(\theta) d\theta, \quad (22)$$

$$A := \iint \prod_{j=1}^n p_\theta(\rho_j)^\beta dm(\rho_j) \pi(\theta) d\theta,$$

is minimized by the Bayesian escort predictive state $\omega_{\pi, \beta}^n$.

Proof. For any measure $\mu = \mu^{\rho^n}$ on $E_{\mathfrak{A}}$ with ϕ^{ρ^n} as its barycenter such that $\mu \ll m$, we have

$$\begin{aligned} S(\omega_\theta \| \psi^{\rho^n}) &= D(\mu_{\omega_\theta} \| \mu) \\ &= \int dm \frac{d\mu_{\omega_\theta}}{dm} \left(\log \frac{d\mu_{\omega_\theta}}{dm} - \log \frac{d\mu}{dm} \right), \end{aligned}$$

and hence,

$$\begin{aligned} &A(T^n(\omega_\theta \| \phi_1^{\rho^n}) - T^n(\omega_\theta \| \phi_2^{\rho^n})) \\ &= \iiint dm \frac{d\mu_{\omega_\theta}}{dm} \left(\log \frac{d\mu_2^{\rho^n}}{dm} - \log \frac{d\mu_1^{\rho^n}}{dm} \right) \prod_{j=1}^n p_\theta(\rho_j)^\beta dm(\rho_j) \pi(\theta) d\theta \\ &= \iint dm \left(\int \frac{d\mu_{\omega_\theta}}{dm} \prod_{j=1}^n p_\theta(\rho_j)^\beta \pi(\theta) d\theta \right) \left(\log \frac{d\mu_2^{\rho^n}}{dm} - \log \frac{d\mu_1^{\rho^n}}{dm} \right) \prod_{j=1}^n dm(\rho_j), \end{aligned}$$

for any $\phi_1^{\rho^n} = b(\mu_1^{\rho^n})$, $\phi_2^{\rho^n} = b(\mu_2^{\rho^n}) \in E_{\mathfrak{A}}$ such that $\mu_1^{\rho^n}, \mu_2^{\rho^n} \ll m$. Now we put $\tau := \frac{1}{B} \int \mu_{\omega_\theta} \prod_{j=1}^n p_\theta(\rho_j)^\beta \pi(\theta) d\theta$ with $B := \int \prod_{j=1}^n p_\theta(\rho_j)^\beta \pi(\theta) d\theta$. If $\frac{d\mu_2^{\rho^n}}{dm}$ is equal to $\frac{d\tau}{dm}$, then the above equalities continue to the following form:

$$\begin{aligned} &= B \iint D(\tau \| \mu_1^{\rho^n}) \prod_{j=1}^n dm(\rho_j) \\ &= B \iint S(b(\tau) \| \phi_1^{\rho^n}) \prod_{j=1}^n dm(\rho_j) \geq 0 \end{aligned}$$

for any $\phi_1^{\rho^n} \in E_{\mathfrak{A}}$. Therefore, the risk function $T^n(\omega_\theta \| \phi^{\rho^n})$ is minimized at the unique state $\phi^{\rho^n} = b(\tau) = \omega_{\pi, \beta}^n$. \square

This theorem is a generalization of [1] and [29], and explains the reason why the Bayesian escort predictive state is a good estimator for a “true” one.

Now we discuss the situations with singular statistics. The results here are proved originally in [33, 34, 35]. The reason why we use this method will be explained in Section 4. For a model $\{\omega_\theta\}_{\theta \in \Theta}$ and a “true” state $\psi \in E_{\mathfrak{A}}$ we assume that there is a subcentral measure m satisfying $\mu_{\omega_\theta}, \mu_\psi \ll m$ and

$$\overline{\left\{ \rho \in E_{\mathfrak{A}} \mid p(\rho|\theta) := p_\theta(\rho) = \frac{d\mu_{\omega_\theta}}{dm}(\rho) > 0 \right\}} = \overline{\left\{ \rho \in E_{\mathfrak{A}} \mid q(\rho) := \frac{d\mu_\psi}{dm}(\rho) > 0 \right\}}$$

for every $\theta \in \Theta$, and we consider

$$L(\theta) := - \int dm(\rho) q(\rho) \log p(\rho|\theta). \quad (23)$$

We assume that there exists at least one parameter $\theta \in \Theta$ that minimizes $L(\theta)$,

$$L_0 = \min_{\theta \in \Theta} L(\theta) \quad (24)$$

and that $p_0(\rho) := p(\rho|\theta_0)$ is one and the same density function for any $\theta_0 \in \Theta_0 := \{\theta \in \Theta \mid L(\theta) = L_0\}$, and we put $\omega_0 := \omega_{\theta_0}$. Then, from such definitions as

$$f(\rho, \theta) := \log \frac{p_0(\rho)}{p(\rho|\theta)}, \quad (25)$$

$$D(\theta) := \int dm(\rho) q(\rho) f(\rho, \theta), \quad (26)$$

$$D_n(\theta) := \frac{1}{n} \sum_{j=1}^n f(\rho_j, \theta), \quad (27)$$

it immediately follows that

$$D(\theta) = S(\psi|\omega_\theta) - S(\psi|\omega_0), \quad (28)$$

$$D_n(\theta) = S_n(\psi|\omega_\theta) - S_n(\psi|\omega_0), \quad (29)$$

where $S_n(\psi|\omega_\theta) = \frac{1}{n} \sum_{j=1}^n \log \frac{q(\rho_j)}{p(\rho_j|\theta)}$. Therefore, we see $D(\theta) \geq 0$.

Assumptions. (1) The open kernel Θ° of the set Θ of parameters θ is non-empty. The boundary of Θ is defined by real analytic functions $\varrho_j(\theta)$ so that

$$\Theta = \{\theta \in \mathbb{R}^d \mid \varrho_1(\theta) \geq 0, \varrho_2(\theta) \geq 0, \dots, \varrho_k(\theta) \geq 0\}. \quad (30)$$

(2) The a priori distribution $\pi(\theta)$ is factorized into the product,

$$\pi(\theta) = \pi_1(\theta) \pi_2(\theta), \quad (31)$$

of a real analytic function $\pi_1(\theta) \geq 0$ and of a function of C^∞ -class $\pi_2(\theta) > 0$.

(3) The map $\Theta \ni \theta \mapsto f(\rho, \theta)$ is an $L^s(q)$ -valued analytic function, where $L^s(q)$ with $s \geq 6$ is defined by

$$L^s(q) := \left\{ f(\rho) \mid \|f\|_s := \left(\int |f(\rho)|^s q(\rho) dm(\rho) \right)^{1/s} < \infty \right\}. \quad (32)$$

(4) There is an $\epsilon > 0$ such that

$$\int \left(\sup_{\theta \in \Theta} |f(\rho, \theta)|^2 \right) \left(\sup_{D(\theta) < \epsilon} p(\rho|\theta) \right) dm(\rho) < \infty. \quad (33)$$

The pair (ψ, ω_θ) is said to be coherent if there exist $A > 0$ and $\epsilon > 0$ such that

$$\theta \in \Theta_\epsilon \Rightarrow S(\psi||\omega_\theta) - S(\psi||\omega_0) \geq A \cdot S(\omega_0||\omega_\theta), \quad (34)$$

where $\Theta_\epsilon := \{\theta \in \Theta | S(\omega_0||\omega_\theta) \leq \epsilon\}$ and, otherwise, incoherent.

In the rest of this subsection, we assume the following condition to hold, in addition to the above assumptions (1) – (4):

Matching Condition 3. *The pair (ψ, ω_θ) satisfies the coherence condition.*

We note that the validity of these assumptions means the interplay between positivity and analyticity which is closely related with the modular structure inherent in the standard form of a von Neumann algebra.

The inequality in (34) can be written as follows:

$$\int dm(\rho) q(\rho) \log \frac{p_0(\rho)}{p(\rho|\theta)} \geq A \cdot D(p_0||p_\theta) \quad (35)$$

for every $\theta \in \Theta_\epsilon$, and the following inequality holds:

$$t + e^{-t} - 1 \geq B(\eta)t^2 \quad (36)$$

for $|t| < \eta$, where $B(\eta)$ is a monotone decreasing strictly positive function of $\eta > 0$. Thus, by fixing η sufficiently large, it holds that

$$L(\theta) - L_0 \geq C \int dm(\rho) p_0(\rho) f(\rho, \theta)^2 \quad (C > 0), \quad (37)$$

for every $\theta \in \Theta_\epsilon$. We can prove the next theorem by using the same methods as in [35]:

Theorem 2.9. *By the resolution of singularities, the functions in Eqs. (26), (25), (27) can be reduced to the following “standard forms”:*

$$D(g(u)) = u^{2k} = u_1^{2k_1} \dots u_d^{2k_d}, \quad (38)$$

$$f(\rho, g(u)) = a(\rho, u)u^k, \quad (39)$$

$$D_n(g(u)) = u^{2k} - \frac{1}{\sqrt{n}} u^k \xi_n(u), \quad (40)$$

where $u = (u_1, \dots, u_d)$ is a coordinate system of an analytic manifold U , and g is an analytic map from U to Θ , k_1, \dots, k_d are non-negative integers, $a(\rho, u)$ is an analytic function on U for each $\rho \in \text{supp } \mu_{\omega_\theta}$ such that $E_\rho[a(\rho, u)] = u^k$, and $\{\xi_n\}$ is an empirical process such that

$$\xi_n(u) = \frac{1}{\sqrt{n}} \sum_{j=1}^n \{a(\rho_j, u) - u^k\}, \quad (41)$$

converges weakly to the Gaussian process $\xi(u)$ with expectation $E_\xi[\xi(u)] = 0$ and covariance $E_\xi[\xi(u)\xi(v)] = E_\rho[a(\rho, u)a(\rho, v)] - u^k v^k$.

The universal validity of the above standard forms of the quantum relative entropy and of the log likelihood ratio function, respectively, is guranteed independently of the model by this theorem.

Furthermore, we need the following theorem proved in [33], as a next step to Theorem 2.9, under the above assumptions:

Theorem 2.10 ([33]). (1) *The set of parameters $\mathcal{U} = g^{-1}(\Theta_\epsilon)$ is covered by a finite set*

$$\mathcal{U} = \bigcup_{\alpha} U_{\alpha},$$

where U_{α} is given by a local coordinate,

$$U_{\alpha} = [0, b]^d = \{(u_1, u_2, \dots, u_d) \mid 0 \leq u_1, u_2, \dots, u_d \leq b\}.$$

(2) *In each U_{α} ,*

$$D(g(u)) = u^{2k} = u_1^{2k_1} \dots u_d^{2k_d},$$

where k_1, \dots, k_d are non-negative integers.

(3) *There is a positive function $\tilde{\pi}(u)$ of class C^∞ such that*

$$\pi(g(u))|g'(u)| = \tilde{\pi}(u)u^h = \tilde{\pi}(u)u_1^{h_1}u_2^{h_2} \dots u_d^{h_d}, \quad (42)$$

where $|g'(u)|$ is the absolute value of the Jacobian determinant and h_1, \dots, h_d are non-negative integers and

$$\tilde{\pi}(u) > c > 0,$$

is a function of class C^∞ , where $c > 0$ is a positive constant.

(4) *There exist a set of functions $\{\sigma_{\alpha}(u)\}$ of class C^∞ which satisfy*

$$\sigma_{\alpha}(u) \geq 0, \quad \sum_{\alpha} \sigma_{\alpha}(u) = 1,$$

$$\sigma_{\alpha}(u) > 0 \ (u \in [0, b]^d), \quad \text{supp } \sigma_{\alpha}(u) = [0, b]^d,$$

such that, for arbitrary integrable function $H(\theta)$,

$$\begin{aligned} \int_{\Theta_\epsilon} H(\theta)\pi(\theta)d\theta &= \int_{\mathcal{U}} H(g(u))\pi(g(u))|g'(u)|du \\ &= \sum_{\alpha} \int_{U_{\alpha}} H(g(u))\tilde{\pi}^*(u)u^h du, \end{aligned}$$

where we define $\tilde{\pi}^*(u)$ by omitting local coordinate α ,

$$\tilde{\pi}^*(u) = \sigma_{\alpha}(u)\tilde{\pi}(u).$$

Proof. See [33]. □

Definition 2.9.

$$Z_n = \int \prod_{j=1}^n p(\rho_j|\theta)^\beta \pi(\theta) d\theta, \quad Z_n^0 = \frac{Z_n}{\prod_{j=1}^n p_0(\rho_j)^\beta} \quad (43)$$

$$F_n = -\frac{1}{\beta} \log Z_n, \quad F_n^0 = -\frac{1}{\beta} \log Z_n^0 \quad (44)$$

Z_n and F_n are called a partition function and a Bayes stochastic complexity, respectively.

The zeta function $\zeta(z) = \int D(\theta)^z \pi(\theta) d\theta$ can be analytically continued to the unique meromorphic function on the entire complex plane. All poles of $\zeta(z)$ are real, negative, rational numbers.

$$(-\lambda) := \text{maximum pole of } \zeta(z) \quad (\lambda > 0), \quad (45)$$

$$m := \text{multiplicity of } (-\lambda). \quad (46)$$

λ and m are called the learning coefficient and its order, respectively. If $D(\theta)$ and a priori distribution $\pi(\theta)$ are represented in Theorem 2.8 and 2.9, then the learning coefficient and its order are given, respectively, by

$$\lambda = \min_{\alpha} \min_{1 \leq j \leq d} \left(\frac{h_j + 1}{2k_j} \right), \quad (47)$$

$$m = \max_{\alpha} \# \{j \mid \lambda = (h_j + 1)/2k_j\}, \quad (48)$$

where $\#$ denotes the cardinality of the set. Let $\{\alpha^*\}$ be a set of all local coordinates in which both the minimization in Eq.(45) and the maximization in Eq.(46) are attained. Such a set of local coordinates $\{\alpha^*\}$ is said to be the essential family of local coordinates. For each local coordinate α^* in the essential family of local coordinates, we assume without loss of generality u is represented as $u = (x, y)$ so that

$$\begin{aligned} x &= (u_1, u_2, \dots, u_m), \\ y &= (u_{m+1}, u_{m+2}, \dots, u_d), \end{aligned}$$

and that

$$\begin{aligned} \lambda &= \frac{h_j + 1}{2k_j} \quad (1 \leq j \leq m), \\ \lambda &< \frac{h_j + 1}{2k_j} \quad (m + 1 \leq j \leq d). \end{aligned}$$

For any function $H(u) = H(x, y)$, we use the notation $H_0(y) := H(0, y)$.

Theorem 2.11. (1)

$$\begin{aligned} &F_n^0 - \frac{\lambda}{\beta} \log n + \frac{m-1}{\beta} \log \log n \\ &\longrightarrow -\frac{1}{\beta} \log \left(\sum_{\alpha^*} \gamma_b \int_0^\infty dt \int_{U_{\alpha^*}} t^{\lambda-1} e^{-\beta t + \beta \sqrt{t} \xi_0(y)} \tilde{\pi}_0^*(y) dy \right) \quad \text{in law.} \end{aligned} \quad (49)$$

(2) *The following asymptotic expansion holds:*

$$F_n = nL_n + \frac{\lambda}{\beta} \log n - \frac{m-1}{\beta} \log \log n + F_n^R, \quad (50)$$

where $L_n = -\frac{1}{n} \sum_{j=1}^n \log p_0(\rho_j)$, and F_n^R is a random variable which converges in law to a random variable.

Proof. We can prove (1) easily by using the same method as used in [33]. We define

$$F_n^R = -\frac{1}{\beta} \log \left(\sum_{\alpha^*} \gamma_b \int_0^\infty dt \int_{U_{\alpha^*}} t^{\lambda-1} e^{-\beta t + \beta \sqrt{t} \xi_{n,0}(y)} \tilde{\pi}_0^*(y) dy \right). \quad (51)$$

Then, (2) immediately derives from (1). \square

This theorem clarifies the behaviour of the Bayes likelihood function which evaluates how close a model approaches to an optimal state, according to the increase of data. Although there is no essential difference between this theorem and that in classical case [33], there is one reason why we described this result here: The results such as Theorem 2.9, 2.11, and the next Theorem 2.12 are the standard objects of interest in modern statistical science, and fundamental analysis in information theory is mainly based on large-deviation type results similar to Theorem 2.11. Therefore, this theorem is of vital importance and need to be investigated in more details regardless of quantum or classical in future.

For a given function $G(\theta)$ on Θ , the a posteriori mean of $G(\theta)$ is defined as

$$\langle G(\theta) \rangle_{\pi, \beta}^{\rho^n} = \frac{\int G(\theta) \prod_{j=1}^n p(\rho_j | \theta)^\beta \pi(\theta) d\theta}{\int \prod_{j=1}^n p(\rho_j | \theta)^\beta \pi(\theta) d\theta}, \quad (52)$$

where $0 < \beta < \infty$. Then, the following equality holds:

$$\omega_{\pi, \beta}^n = \int \rho \langle p(\rho | \theta) \rangle_{\pi, \beta}^{\rho^n} dm(\rho). \quad (53)$$

Definition 2.10.

(1) *Bayes generalization error and Bayes generalization loss are defined, respectively, by*

$$\mathcal{E}_{bg} = E_\rho \left[\log \frac{q(\rho)}{\langle p(\rho | \theta) \rangle_{\pi, \beta}^{\rho^n}} \right], \quad \mathcal{L}_{bg} = E_\rho \left[-\log \langle p(\rho | \theta) \rangle_{\pi, \beta}^{\rho^n} \right]. \quad (54)$$

(2) *Bayes training error and Bayes training loss are defined, respectively, by*

$$\mathcal{E}_{bt} = \frac{1}{n} \sum_{j=1}^n \left[\log \frac{q(\rho_j)}{\langle p(\rho_j | \theta) \rangle_{\pi, \beta}^{\rho^n}} \right], \quad \mathcal{L}_{bt} = \frac{1}{n} \sum_{j=1}^n \left[-\log \langle p(\rho_j | \theta) \rangle_{\pi, \beta}^{\rho^n} \right]. \quad (55)$$

(3) *functional variance is defined by:*

$$\mathcal{V} = \sum_{j=1}^n \left\{ \langle (\log p(\rho_j | \theta))^2 \rangle_{\pi, \beta}^{\rho^n} - (\langle \log p(\rho_j | \theta) \rangle_{\pi, \beta}^{\rho^n})^2 \right\}. \quad (56)$$

These notions are the main targets to be estimated or calculated in statistics and learning theory. We can easily check that

$$\begin{aligned} \mathcal{E}_{bg} &= D(q \| \langle p(\cdot | \theta) \rangle_{\pi, \beta}^{\rho^n}) = S(\psi \| \omega_{\pi, \beta}^n), \\ \mathcal{E}_{bg} &= \mathcal{L}_{bg} + E_\rho [\log q(\rho_j)], \\ \mathcal{E}_{bt} &= \mathcal{L}_{bt} + \frac{1}{n} \sum_{j=1}^n \log q(\rho_j). \end{aligned} \quad (57)$$

Our present concern is the following theorem.

Theorem 2.12.

$$E[\mathcal{L}_{bg}] = E[\text{WAIC}] + o\left(\frac{1}{n}\right), \quad (58)$$

$$\text{WAIC} = \mathcal{L}_{bt} + \frac{\beta}{n}\mathcal{V}. \quad (59)$$

Proof. See [35]. □

WAIC is the acronym for “widely applicable information criteria”. It is shown by this theorem that the WAIC for a central measure is asymptotically equal to the Bayes generalization loss. Since WAIC for $p_\theta = \frac{d\mu_{\omega_\theta}}{dm}$ is a quantum version of the information criteria (IC), this result can be successfully interpreted as establishing IC for quantum states. This also justifies our use of the central measure μ_ω for the central decomposition of $\omega \in E_{\mathfrak{A}}$: namely, owing to the use of central decomposition, our LDS in the second level can determine representations controlling spectra of observables, on the basis of numerical data of such a quantity as WAIC. It is important, not only practically but also conceptually, that such qualitative aspects as representations of the algebra of observables can be estimated by this kind of quantitative data. In addition, WAIC in quantum case should be contrasted with that in classical case, since the latter cannot evaluate representations of the algebra. On the other hand, we note that IC in the first level are the same as those in classical case.

2.3.2 Physical meaning and practical use

We can conclude that we have established the following procedures:

Rate function \Rightarrow Predictive state \Rightarrow Information criterion (\Rightarrow “True” state).

The procedure established in Section 2.3.1 is a typical example of this:

Quantum relative entropy $S(\cdot\|\cdot) \Rightarrow$
Bayesian escort predictive state $\omega_{\pi,\beta}^n \Rightarrow \text{WAIC} = \mathcal{L}_{bt} + \frac{\beta}{n}\mathcal{V}$ (\Rightarrow “True” state ψ).

First, rate functions are specified by procedures in LDP. A rate function is a barometer to what extent one state diverges from a “true” one. Secondly, we construct predictive states from models and data by applying the results of several steps whose starting point is the rate function provided by the first step. Thirdly, we define IC and use it for selecting the best predictive state from candidates. Lastly, we select one state which should be treated as a “true” one ψ in Section 2.3.1. Taking this step, we can reach a “true” state by using the methods in Section 2.3.1 such as Theorem 2.9, 2.11, and 2.12. As stated in Section 2.3.1, IC are estimators for rate functions as quasi-distances from a “true” state to a predictive state, which have bias terms based on the method to construct predictive states.

3 Examples

Once the sector structure consisting of mutually disjoint factor states is clarified, the Micro-Macro duality starts to be valid, according to which the present method of LDS

becomes effective. From this viewpoint, the following examples are instructive in the sense that the method in LDS second level enable us to reduce complicated dynamical systems partially to kinematics.

(1) Non-equilibrium states in quantum field theory

The method established in [6] is used for describing non-equilibrium states in QFT. The universal model of the relevant sector structure to this context is known to be provided by a family of factor KMS (Kubo-Martin-Schwinger) states $\{\omega_{\beta,\mu}|\beta > 0, \mu \in K\}$ on a von Neumann algebra \mathfrak{M} of type III parametrized by the inverse temperature β and by all other necessary thermodynamic parameters denoted collectively by $\mu \in K$ such as a chemical potential. Following the ideas in [6], we can write a non-equilibrium state of the system whose reference states are $\{\omega_{\beta,\mu}|\beta > 0, \mu \in K\}$ on a von Neumann algebra \mathfrak{M} of type III as follows:

$$\omega_{B,\rho} = \int_B d\rho(\beta, \mu) \omega_{\beta,\mu}, \quad (60)$$

where B is a compact subset of $\mathbb{R}_{>0} \times K$ and ρ is a regular Borel measure on $\mathbb{R}_{>0} \times K$. In this situation, we can construct a model $\{\rho_\theta(\beta, \mu)|\theta \in \Theta \subset \mathbb{R}^d : \text{compact}\}$ of probability distribution, in terms of which the method of statistical inference can be systematically applied for the purpose of further developments of the theory of non-equilibrium states in QFT.

(2) Conformal field theory and critical phenomena

Let \mathfrak{C} be a C*-algebra generated by $\{e^{iL_n}, e^{iC}|n \in \mathbb{Z}\}$ such that operators $\{L_n\}$ and a self-adjoint operator C on a Hilbert space \mathfrak{H} satisfy

$$[L_m, L_n] = (m - n)L_{m+n} + \frac{m^3 - m}{12}C\delta_{m+n,0}, \quad [L_n, C] = 0. \quad (61)$$

Let $\{\omega_c|c \in \text{Spec}(C) \subset \mathbb{R}\}$.

$$\omega_R = \int_R d\sigma(c) \omega_c, \quad (62)$$

where σ is a regular Borel measure on $\text{Spec}(C)$ and R is compact subset of $\text{Spec}(C)$. In view of the accumulated applications of conformal field theory, it would be natural to expect the possibility of systematic theory for statistical estimate about critical phenomena in solid state physics on the basis of the mathematical knowledge about the reducible representations and states of this kind, which would be the target for future tasks.

4 Discussion on Quantum Estimation Theory: Quantum Model Selection

In Section 2.3.2, we have discussed estimation theory for quantum states. Remarkably, the methods developed here allow us to take full advantage of the usual measure-theoretical analysis in statistics, information theory and learning theory even for estimation of quantum states in the context of quantum theory, which is due to our bringing the use of the central measure μ_ω of $\omega \in E_{\mathfrak{A}}$ into focus. This should be contrasted with many previous attempts in quantum estimation theory, where vain efforts have been expended for the attempts of formulating new notions or “quantized version” of the notions known in classical (measure-theoretical) statistics, information theory and learning theory. Instead, what is most crucial here is the difference in the method of inference according to whether a state to be estimated is factor or not. Since the methods discussed in Section 2.3 are for

non-factor states, different analysis from the one for factor states need to be built up. On the other hand, we have succeeded in constructing quantum model selection, which is a quantum version of model selection, by using measure-theoretic methods. Model selection began when Akaike introduced the concept of information criteria in 1971 [2, 3] to resolve the insufficiency of hypothesis testing for selecting the best predictive distribution. The best known and used one is the Akaike information criterion (AIC)

$$\text{AIC} = -\frac{1}{n} \sum_{j=1}^n p(x_j | \hat{\theta}_{MLE}) + \frac{d}{n} \quad (63)$$

where $\hat{\theta}_{MLE}$ is the maximal likelihood estimator (MLE) and d is the dimension of parameters. AIC can be applied in the situation that the maximal likelihood method, or the M-estimation method, is used for regular models. Furthermore, WAIC appearing in singular statistics [33, 34] is another version of IC and contains AIC and TIC as a special case. Roughly speaking, model selection is the method for selecting the predictive distribution which attains the minimum of IC in several candidates. Although AIC has been used for quantum states in [32, 36], the reason has not been clarified why we can apply it for quantum states. Because they applied AIC to a general positive operator-valued measure (POVM), not to PVM's, their use is not precisely in the first level. However, with the help of measuring processes and Naimark dilation, we can justify their use. Thus it is desirable to examine the validity of the use of IC for quantum states.

Remark 4.1. *It is occasionally said that, by using AIC, or BIC, some model with fewer parameters is automatically chosen. However, this statement is not precise and is no more than hindsight: if two models have almost equal training errors, then AIC of the model with fewer parameters becomes smaller than the others, and the model having the smallest AIC is naturally chosen. As stated in Section 2.3.2, we should fix a “true” state by using the predictive state and test the performance of the latter compared with other predictive states. Therefore, we should use flexibly the predictive state selected by IC without taking it by absolute priority.*

In recent years, algebraic geometry and algebraic analysis are successfully applied to the singular aspects in learning theory. Many statistical models, such as the normal mixture model

$$f(x|\mathbf{a}, \mathbf{b}, \mathbf{c}) = \sum_{j=1}^M a_j \varphi(x|b_j, c_j), \quad (64)$$

where $\mathbf{a} = (a_1, \dots, a_M)$ such that $a_1, \dots, a_M \geq 0$ and $\sum_{j=1}^M a_j = 1$, $\mathbf{b} = (b_1, \dots, b_M) \in \mathbb{R}^M$, $\mathbf{c} = (c_1, \dots, c_M) \in (\mathbb{R}_+)^M$ and $\varphi(x|b, c) = \frac{1}{(2\pi c^2)^{1/2}} \exp \left\{ -\frac{1}{2c^2} (x - b)^2 \right\}$, have degenerate Fisher information matrices, so that Riemannian-geometric methods cannot be applied. Then the Cramér-Rao inequality

$$V(\theta) \geq J^{-1}(\theta), \quad (65)$$

does not hold without any significance, where $V(\theta) = (E_x[(\hat{\theta}_j(x) - \theta_i)(\hat{\theta}_j(x) - \theta_j)])_{i,j}$ and $J^{-1}(\theta)$ are, respectively, the covariance matrix for $\theta = (\mathbf{a}, \mathbf{b}, \mathbf{c})$ and the inverse of the Fisher information matrix $J(\theta)$. Therefore, different methods using algebraic geometry and algebraic analysis are investigated, which work efficiently in various areas, and

are already used in a textbook [8], which has encouraged us to use algebraic geometric methods.

Lastly, we give a generalization of quantum hypothesis testing. Suppose that $\varphi, \psi \in E_{\mathfrak{A}}$ have central measures given, for any integrable function f , by

$$\begin{aligned}\int f(\rho) d\mu_{\varphi}(\rho) &= \sum_{j=1}^m \alpha_j f(\rho_j), \\ \int f(\rho) d\mu_{\psi}(\rho) &= \sum_{j=1}^m \beta_j f(\rho_j),\end{aligned}$$

with $\sum_j \alpha_j = \sum_j \beta_j = 1$, $0 < \alpha_j, \beta_j < 1$ ($j = 1, \dots, m$), corresponding, respectively, to the following diagonal matrices:

$$\mu_{\varphi} \leftrightarrow \sigma_{\varphi} = \begin{pmatrix} \alpha_1 & & & O \\ & \alpha_2 & & \\ & & \ddots & \\ O & & & \alpha_m \end{pmatrix}, \quad \mu_{\psi} \leftrightarrow \sigma_{\psi} = \begin{pmatrix} \beta_1 & & & O \\ & \beta_2 & & \\ & & \ddots & \\ O & & & \beta_m \end{pmatrix}. \quad (66)$$

Let $E_{\psi}(\Delta)$ ($\Delta \in \mathcal{B}(\text{supp } \mu_{\psi})$) be the PVM corresponding to μ_{ψ} (see Eq.(14)). It is immediately seen that $S(\varphi\|\psi) = D(\mu_{\varphi}\|\mu_{\psi}) = S(\sigma_{\varphi}\|\sigma_{\psi})$. We treat the state ψ as a “true” one and assume that a test function of interest $S^n : (\text{supp } \mu_{\psi})^n \mapsto \{0, 1\}$. S^n has a positive operator representation A_n on $M(m, \mathbb{C})^{\otimes n}$ such that $0 \leq A_n \leq I_{M(m, \mathbb{C})^{\otimes n}}$. Then, the error probabilities of the first kind and the second kind can, respectively, be defined by

$$\begin{aligned}\alpha_n(A_n) &= \text{Tr}[\sigma_{\psi}^{\otimes n}(I - A_n)], \\ \beta_n(A_n) &= \text{Tr}[\sigma_{\varphi}^{\otimes n} A_n].\end{aligned}$$

The following theorem is a generalization of quantum Stein’s lemma and can be proved by the same method as found in [15, 21, 12], valid for the version of quantum Stein’s theorem in these papers.

Theorem 4.1. *For any $0 < \epsilon < 1$, it holds that*

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log \beta_n^*(\epsilon) = -S(\psi\|\varphi), \quad (67)$$

where $\beta_n^*(\epsilon)$ is the minimum second error probability under the constraint that the first error probability is less than ϵ , i.e.,

$$\beta_n^*(\epsilon) = \{\beta_n(A_n) | A_n \in M(m, \mathbb{C})^{\otimes n}, 0 \leq A_n \leq I_{M(m, \mathbb{C})^{\otimes n}}, \alpha_n(A_n) \leq \epsilon\}. \quad (68)$$

It is important that $\{A_n\}$ are merely operator-valued representations of tests $\{S_n\}$ without actual uses in measurements, where $E_{\psi}(\Delta)$ is actually used. It is obvious that the quantum relative entropy formulated in the present paper is accessible to actual experimental situations whose operational meaning is different from that in [12, 15, 20, 21] formulated in quantum i.i.d. states.

5 Conclusion and Perspective

In this paper we have proposed Large Deviation Strategy and established its first and second levels. For this purpose, we have clarified that the quantum relative entropy plays the role of the rate function in LDP 2nd level, according to which several measure-theoretical methods work efficiently in quantum case.

While results of this sort have been anticipated on the basis of a simple analogy to the classical case or direct computations in some special situations, the pertinence of such formal derivations has been questionable for lack of the appropriate operational setting-up to guarantee the appropriate interpretation. In the present case, we can safely use the natural relation, $S(\psi\|\omega) = D(\nu\|\mu)$, due to [14] to bridge the quantum context with the classical one, which sweeps away all the suspicions.

However, the situation about the estimation theory for the internal structures of a factor state is quite different, which seems to require some new ideas. For this purpose, the measurement scheme formulated in [24, 11] would be instructive as its aim is to search the internal structure of a factor state. To proceed further along the present line of thoughts, the tasks to construct estimation theory for factor states and to establish the third and fourth levels in LDS will be crucially important.

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A Barycentric Decomposition of States and Extension of Algebra

In the barycentric decomposition, $\omega = \int_{E_{\mathfrak{A}}} \rho \, d\mu(\rho)$, of a state ω of \mathfrak{A} by an orthogonal measure μ we have a spectral measure $E_\mu := (\mathcal{B}(\text{supp } \mu) \ni \Delta \mapsto E_\mu(\Delta) := \kappa_\mu(\chi_\Delta) \in \mathfrak{B})$ on $E_{\mathfrak{A}}$, taking values in a subalgebra \mathfrak{B} of the commutant $\pi_\omega(\mathfrak{A})'$ but not in $\pi_\omega(\mathfrak{A})''$ of observables. When we consider a physical process described by this spectral measure, it involves the object system with $\pi_\omega(\mathfrak{A})'' (\subset L^\infty(E_{\mathfrak{A}}, \mu))$ and the measuring one $\mathfrak{B} (\subset \pi_\omega(\mathfrak{A})')$, the latter of which registers the indices to determine states of \mathfrak{A} . According to the measurement scheme [24, 11], we have a composite system consisting of these two algebras $\pi_\omega(\mathfrak{A})''$ and \mathfrak{B} through a suitable measurement coupling, which amounts to the extension of algebra:

$$\pi_\omega(\mathfrak{A})'' \hookrightarrow \pi_\omega(\mathfrak{A})'' \vee \mathfrak{B} \cong \pi_\omega(\mathfrak{A})'' \otimes \mathfrak{B} \subset \pi_\omega(\mathfrak{A})'' \vee \pi_\omega(\mathfrak{A})' = \mathfrak{Z}_{\pi_\omega}(\mathfrak{A})'. \quad (69)$$

In this context, we can extend the state $\omega \in E_{\mathfrak{A}}$ to the one $\tilde{\omega}$ on the algebra $\pi_\omega(\mathfrak{A})'' \vee \mathfrak{B}$ simply defined for $A \in \pi_\omega(\mathfrak{A})'' \vee \mathfrak{B}$ by

$$\tilde{\omega}(A) = \langle \Omega_\omega, A \Omega_\omega \rangle. \quad (70)$$

The naturality of this procedure is understood in relation with Tomita-Takesaki modular theory [5, 28], which plays vital roles in LDS 2nd level to define the quantum relative entropy. Here we note also that \mathfrak{B} is an abelian subalgebra of $\pi_\omega(\mathfrak{A})'$ and that $\pi_\omega(\mathfrak{A})' = J\pi_\omega(\mathfrak{A})''J$ in terms of the modular conjugation operator J which lives in the standard representation of $\pi_\omega(\mathfrak{A})''$. The most important barycentric measures apart from central ones are extremal measures corresponding to a maximal abelian subalgebra of $\pi_\omega(\mathfrak{A})'$. The measure μ is pseudosupported by the pure states $\mathcal{E}(E_{\mathfrak{A}})$ over \mathfrak{A} .

Let μ be an orthogonal measure with a barycenter $\psi \in E_{\mathfrak{A}}$ such that there is a subcentral measure m satisfying $\mu \ll m$. By the same discussion as in Section 2.3.1, we define for any $\Gamma \in \mathcal{B}_{cy}(M_1(E_{\mathfrak{A}}))$,

$$Q_n^{(2A)}(\Gamma) = P_\mu(L_n \in \Gamma). \quad (71)$$

Then, the next theorem holds.

Theorem A.1. *Let \mathfrak{A} be a separable C^* -algebra, ψ be a state on \mathfrak{A} , and μ be a barycentric measure of ψ . Then $Q_n^{(2A)}$ satisfies LDP with the rate function $D(\cdot\|\mu) (= S(b(\cdot)\|\psi))$:*

$$\begin{aligned} -\underline{D}(\Gamma\|\mu) &:= -\inf_{\nu \in \Gamma^o} D(\nu\|\mu) \leq \liminf_{n \rightarrow \infty} \frac{1}{n} \log Q_n^{(2A)}(\Gamma) \\ &\leq \limsup_{n \rightarrow \infty} \frac{1}{n} \log Q_n^{(2A)}(\Gamma) \leq -\inf_{\nu \in \bar{\Gamma}} D(\nu\|\mu) =: -\overline{D}(\Gamma\|\mu) \end{aligned} \quad (72)$$

for any $\Gamma \in \mathcal{B}_{cy}(M_1(E_{\mathfrak{A}}))$. If there exists a subcentral measure m such that $\nu, \mu \ll m$, then $D(\nu\|\mu) = S(b(\nu)\|\psi)$ holds for such ν belonging to $\bar{\Gamma}$ (or Γ^o) that $D(\nu\|\mu) = \overline{D}(\Gamma\|\mu)$ or $\underline{D}(\Gamma\|\mu)$.

The results in Section 2.3.1 and Section 4 also hold for general barycentric measures. It is, however, necessary to keep in mind that barycentric decompositions in general do not always have clear physical meaning, in contrast to a central decomposition. To extend quantum estimation theory this point has to be resolved.

References

- [1] J. Aitchison, Goodness of prediction fit, *Biometrika* **62**, 547-554 (1975).
- [2] H. Akaike, Information theory and an extension of the maximum likelihood principle, in: B.N. Petrov and F. Csaki, eds., 2nd international symposium on information theory (Akademiai Kiado, Budapest, 1973).
- [3] H. Akaike, A new look at the statistical model identification, *IEEE Trans. Automatic Control* **19**, 716-723 (1974).
- [4] S. Amari and H. Nagaoka, *Methods of Information Geometry*, Translations of mathematical monographs; v. 191, Amer. Math. Soc. & Oxford Univ. Press (2000).
- [5] O. Bratteli and D.W. Robinson, *Operator Algebras and Quantum Statistical Mechanics* (vol.1) (2nd printing of 2nd ed.), (Springer, 2002).
- [6] D. Buchholz, I. Ojima and H. Roos, Thermodynamic properties of nonequilibrium states in quantum field theory, *Ann. Phys. (N.Y.)* **297**, 219-242 (2002).

- [7] A. Dembo and O. Zeitouni, *Large deviations techniques and applications* (2nd ed.), (Springer, 2002).
- [8] M. Drton, B. Sturmfels, and S. Sullivant, *Lectures on Algebraic Statistics*, (Birkhäuser, 2008).
- [9] R.S. Ellis, *Entropy, Large Deviations, and Statistical Mechanics*, (Springer, 1985).
- [10] M. Enock and J.-M. Schwartz, *Kac Algebras and Duality of Locally Compact Groups*, (Springer, 1992).
- [11] R. Harada and I. Ojima, A unified scheme of measurement and amplification processes based on Micro-Macro Duality –Stern-Gerlach experiment as a typical example–, *Open Sys. Inform. Dyn.* **16**, 55-74 (2009).
- [12] *Asymptotic Theory of Quantum Statistical Inference*, edited by M. Hayashi (World Scientific, Singapore, 2005).
- [13] C.W. Helstrom, *Quantum Detection and Estimation Theory* (Academic Press, New York, 1976).
- [14] F. Hiai, M. Ohya and M. Tsukada, Sufficiency and relative entropy in $*$ -algebras with applications in quantum systems, *Pacific J. Math.* **107**, 117-140 (1983).
- [15] F. Hiai and D. Petz, The proper formula for relative entropy and its asymptotics in quantum probability, *Commun. Math. Phys.* **143**, 99-114 (1991).
- [16] S. Holevo, *Probabilistic and Statistical Aspects of Quantum Theory* (North-Holland, Amsterdam, 1982).
- [17] M.G. Krein, A duality principle for bicomact groups and quadratic block algebras, *Doklady Akad. Nauk SSSR* **69** (1949), 725-728.
- [18] S. Mac Lane, *Categories for the Working Mathematician* (2nd ed.), (Springer, New York, 1998).
- [19] M. Nielsen, and I. Chuang, *Quantum Computation and Quantum Information*, (Cambridge Univ. Press, 2000).
- [20] T. Ogawa and M. Hayashi, On error exponents in quantum hypothesis testing, *IEEE Trans. Inform. Theory* **50**, 1368-1372 (2004)
- [21] T. Ogawa and H. Nagaoka, Strong converse and Stein’s lemma in quantum hypothesis testing, *IEEE Trans. Inform. Theory* **46**, 2428-2433 (2000).
- [22] I. Ojima, Order Parameters in QFT and Large Deviation (in Japanese), *RIMS Kyokuyuroku* **1066** (1998), 121–132.
- [23] I. Ojima, A unified scheme for generalized sectors based on selection criteria – Order parameters of symmetries and of thermality and physical meanings of adjunctions –, *Open Sys. Inform. Dyn.* **10**, 235-279 (2003).
- [24] I. Ojima, “Micro-Macro Duality in Quantum Physics”, pp.143-161 in *Proc. Intern. Conf. on Stochastic Analysis, Classical and Quantum* (World Scientific, 2005), arXiv:math-ph/0502038.

- [25] I. Ojima, Meaning of Non-Extensive Entropies in Micro-Macro Duality, J. Phys.: Conf. Ser. **201** (2010) 012017.
- [26] I. Ojima, Space(-Time) Emergence as Symmetry Breaking Effect, Invited talk at International Conference in QIBC (= Quantum Bio-Informatics Center, Tokyo University of Sciences) 2010, arXiv:math-ph/1102.0838; Micro-Macro Duality and Space-Time Emergence, Invited talk at International Conference, “Advances in Quantum Theory” at Linnaeus University, June 2010.
- [27] M. Ohya and D. Petz, *Quantum Entropy and Its Use*, (Springer, Berlin, 1993).
- [28] M. Takesaki, *Theory of Operator Algebras II*, (Springer, 2002).
- [29] F. Tanaka and F. Komaki, Bayesian predictive density operators for exchangeable quantum-statistical models, Phys. Rev. A **71**, 052323 (2005).
- [30] T. Tannaka, Über den Dualitätssatz der nicht kommutativen topologischen Gruppen, Tôhoku Math. J. **45** (1938), 1-12.
- [31] N. Tatsuuma, A duality theory for locally compact groups, J. Math. Kyoto Univ. **6**, 187-217 (1967).
- [32] K. Usami, Y. Nambu, Y. Tsuda, K. Matsumoto and K. Nakamura, Accuracy of quantum-state estimation utilizing Akaike’s information criterion, Phys. Rev. A **68**, 022314 (2003).
- [33] S. Watanabe, *Algebraic geometry and statistical learning theory*, (Cambridge University Press, 2009).
- [34] S. Watanabe, Asymptotic learning curve and renormalizable condition in statistical learning theory, J. Phys.: Conf. Ser. **233** (2010) 012014.
- [35] S. Watanabe, Asymptotic Equivalence of Bayes Cross Validation and Widely Applicable Information Criterion in Singular Learning Theory, , J. of Mach. Lear. Res. **11**, 3571-3591, (2010).
- [36] J.O.S. Yin and S.J. van Enk, Information criteria for efficient quantum state estimation, Phys. Rev. A **83**, 062110 (2011).